

Supplementary data

One-step assisted extraction of patulin – a new LC-MS/MS method for testing apples and apple products

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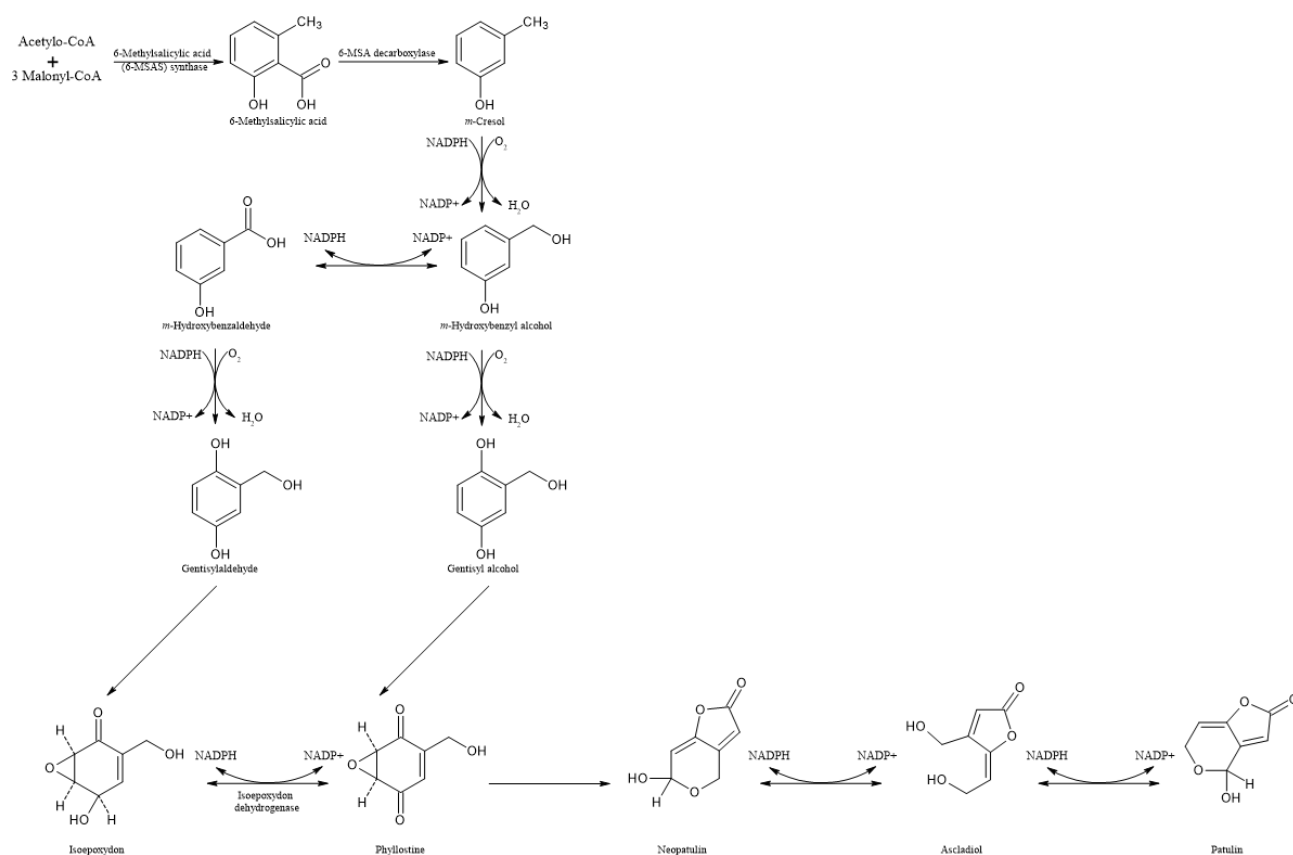


Figure S1. Patulin biosynthesis pathway. Authors' preparation based on (Câmara et al., 2023).

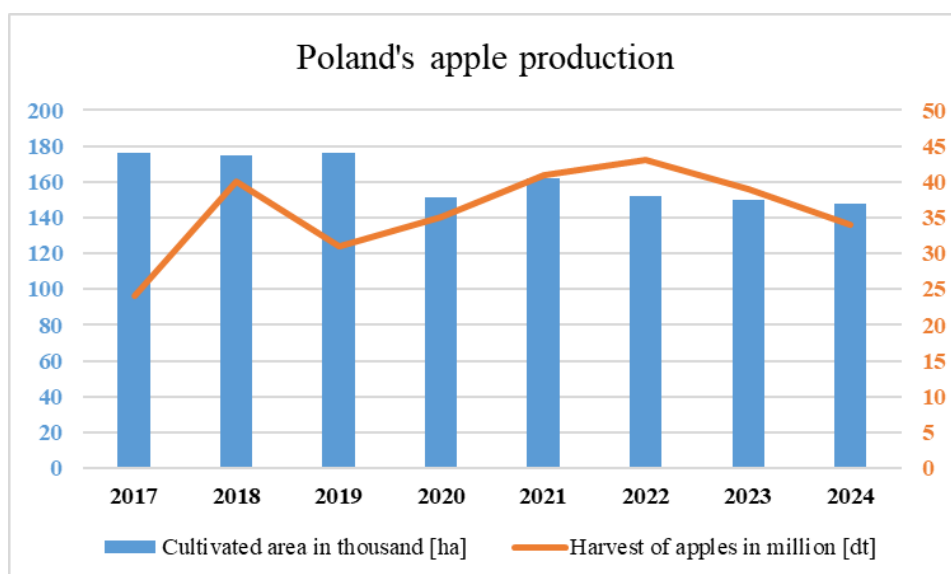


Figure S2. Apple production in Poland 2017-2023. Authors' preparation based on (*Główny Urząd Statystyczny / Obszary Tematyczne / Rolnictwo. Leśnictwo / Uprawy Rolne i Ogrodnicze / Wstępna Ocena Przechowywania Upraw Oзимych w 2010 r., n.d.; Jabłka - Ministerstwo Rolnictwa i Rozwoju Wsi - Portal Gov.Pl, n.d.*).

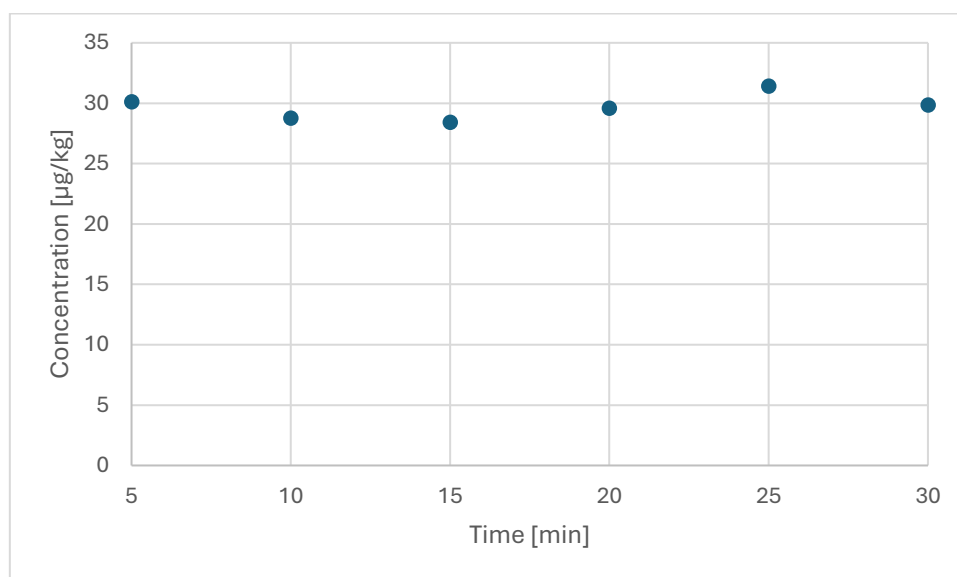


Figure S3. Extraction efficiency of PAT as a function of shaking time.

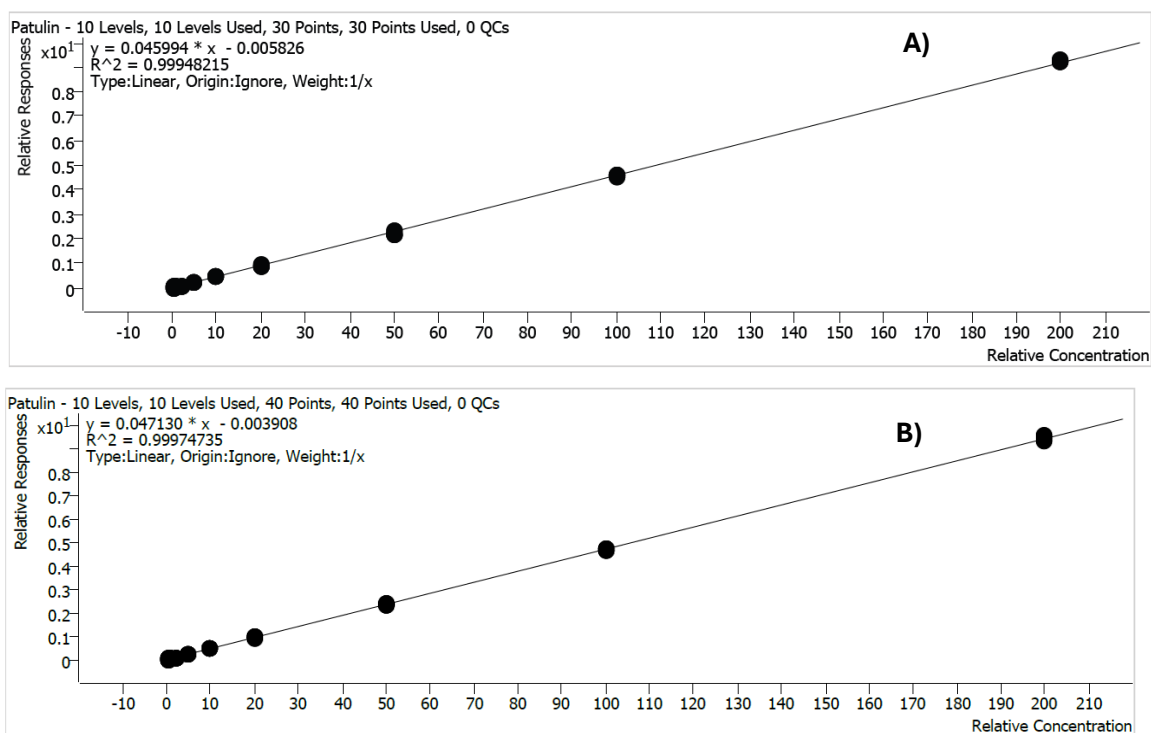


Figure S4. Calibration curves. A) Intraday. B) Interday.

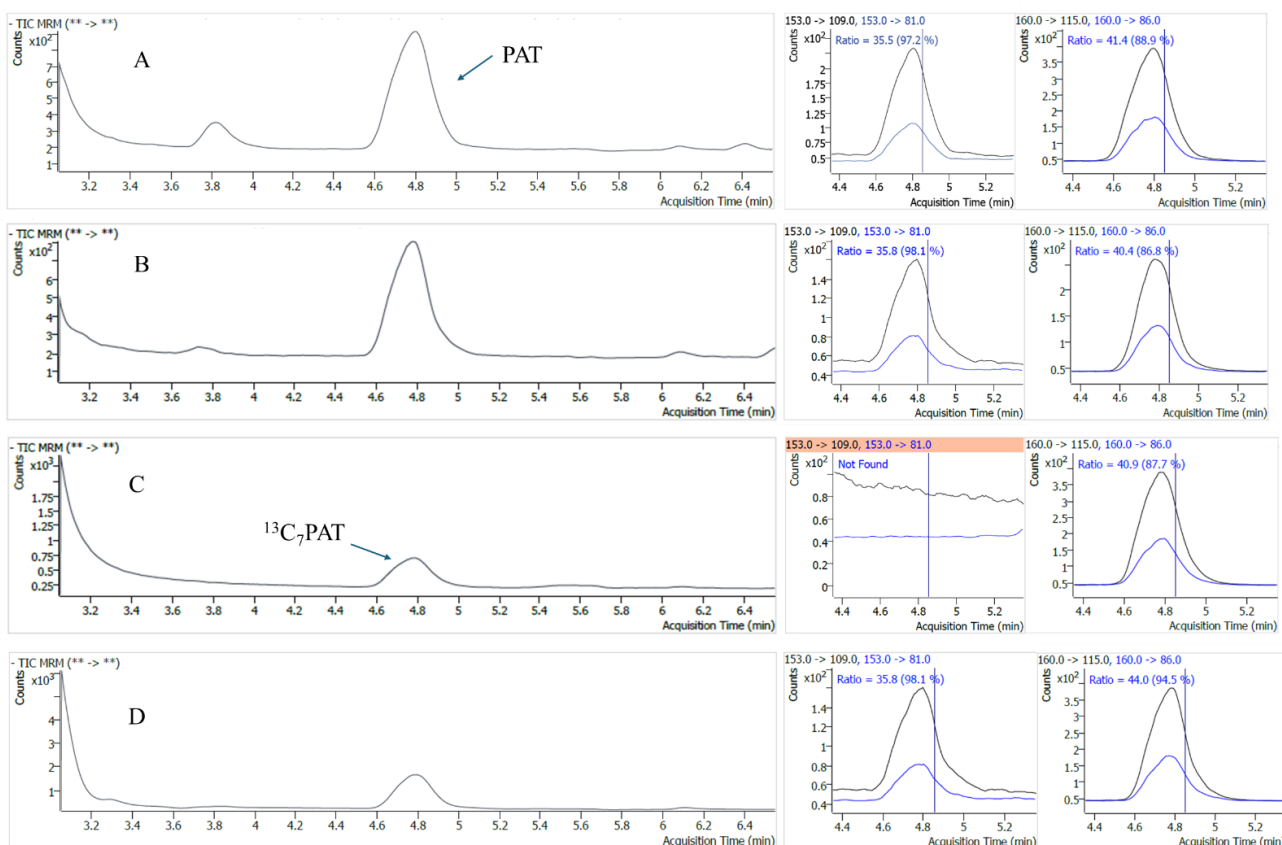


Figure S5. Figure S5. Chromatograms for: A - fortified 10 µg/kg apple mousse, B - proficiency test materials with assigned target values and acceptable ranges as reference materials, C - apple juice for children, D - fortified 10 µg/kg smoothie

Table S1. ESI source parameters for tandem mass spectrometry.

Parameters	Values from Optimizer	Values after manual selection
Dry gas temperature [°C]	150	200
Dry gas flow [L/min]	6	8
Nebulizer pressure [psi]	60	60
Sheath gas temperature [°C]	350	350
Sheath gas flow [L/min]	10	10
Capillary [V]	2000	3000
Nozzle voltage [V]	0	0

Table S2. Validation data for standard solutions.

Concentrations	Intraday		Interday	
[µg/L]	precision [%]	accuracy [%]	precision [%]	accuracy [%]
0.25	6.3	101.7	8.8	102.0
0.5	9.3	99.7	7.8	94.5
1	4.3	101.0	5.4	103.8
2	2.2	99.3	7.2	99.7
5	2.8	99.1	2.4	96.6
10	2.8	102.9	4.9	103.3
20	6.7	96.5	7.6	100.6
50	4.0	99.7	1.8	99.8
100	1.4	99.5	1.4	99.9
200	0.1	100.5	1.1	100.0

Table S3. Different approaches to the analysis of PAT in food using the LC-MS/MS technique.

Type of samples	Sample preparation method	Accuracy [%]	LOQ [$\mu\text{g/kg}$]	Ref.
soft fruits	QuEChERS type extraction with dSPE and sample concentration	50.25-82.37	0.65-3.01 ^a	(Sadok et al., 2023)
apple jam, apple concentrate, apple juice, ground apple	extraction with ethyl acetate, evaporated and reconstituted, SPE	98.32-100.83	0.8-2.4 ^a	(Seo et al., 2015)
fruit juice and dried fruit	extraction with methanol, in-tube SPME	88.3-96.7	0.0705 $\mu\text{g/L}$	(Kataoka et al., 2009)
juice: apple, mango, pineapple, guava, lychee, tamarind, soursop, mixed fruit,	extraction with ethyl acetate, evaporated and reconstituted	99.8-106	0.76 $\mu\text{g/L}$	(Lee et al., 2014)
apple juice	QuEChERS type extraction	92-103	1.15	(Câmara et al., 2023)
fruit and their product: apples, pears, strawberries, apricots, peaches, bananas, grape vines; plums, raspberries, blueberries, blackberries, sour cherries, mix fruit salad	QuEChERS type extraction and SPE	92-109	1-2.5 ^a	(Vaclavikova et al., 2015)
apple, apple juice	extraction with ethyl acetate, dSPE, sample concentration	76-108	42	(Dias et al., 2019)
maize	QuEChERS type extraction with dSPE	66.9-105.8	4.5	(Leite et al., 2023)
apple products: juice and apple puree	extraction with ethyl acetate, evaporated and reconstituted	95.3-99.1	10	(Rosinská et al., 2009)

^a LOQ various for different matrices

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